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Length Scales and Time Scales in Peridynamics

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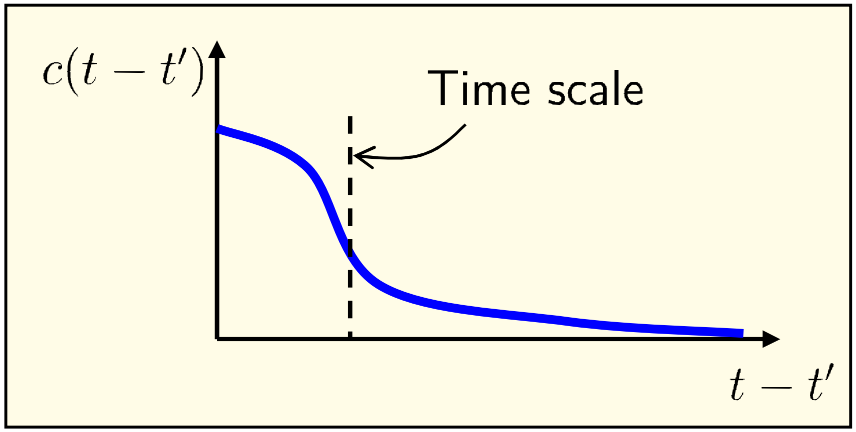
Should a material model have a time scale? (1) Homogeneous

- Some materials have a response that is clearly time-dependent. Example: viscoelasticity can be modeled using nonlocality in time:

$$\sigma(t) = E\varepsilon(t) + \int_0^t c(t-t')\dot{\varepsilon}(t')\,dt'$$

where σ=stress, ε=strain, E is a constant, and c is a (measurable) relaxation function.



- The transition from stochastic processes to continua (e.g., Mori-Zwanzig) can also produce *memory terms*.

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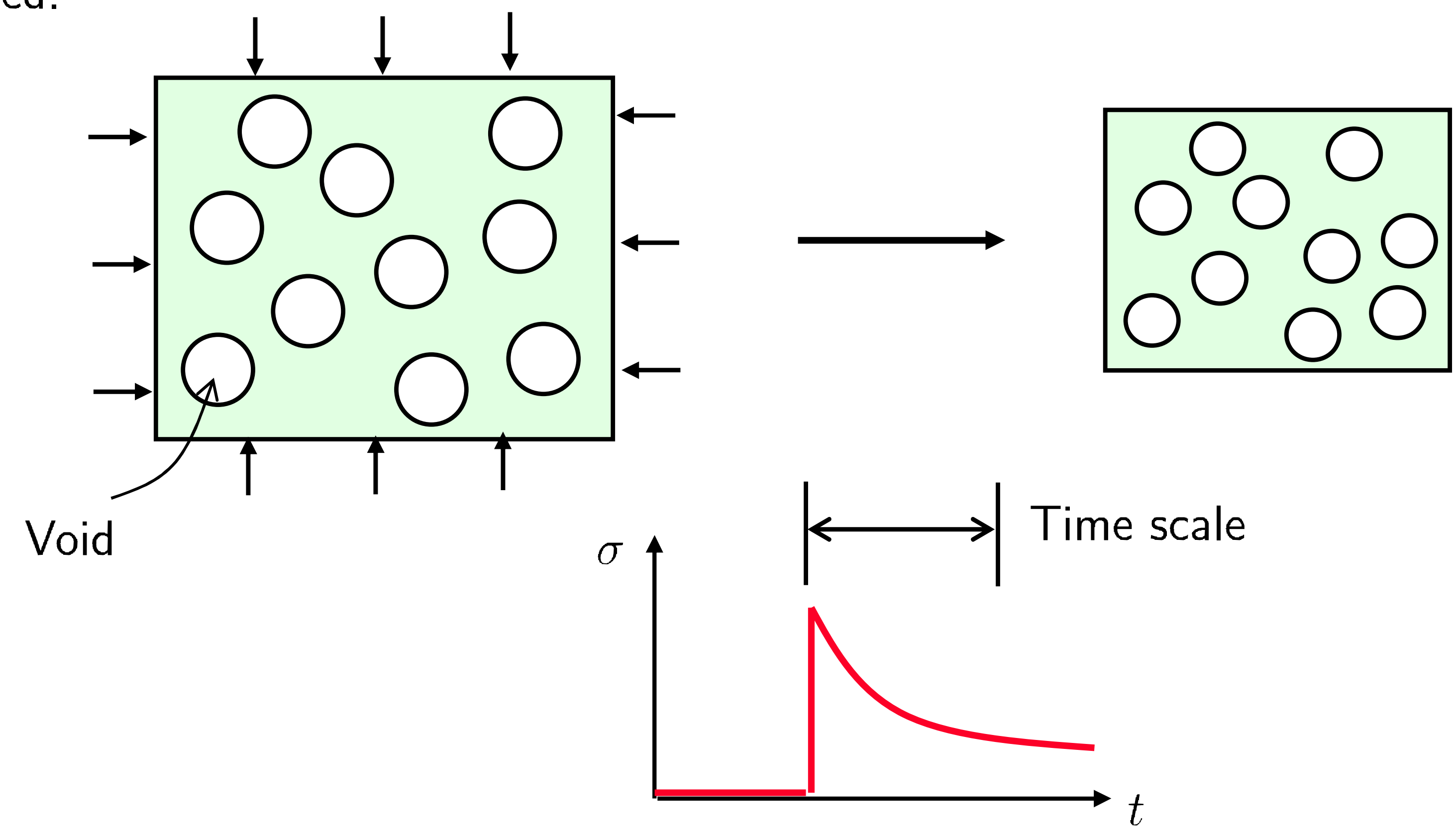
Should a material model have a time scale?
(2) Heterogeneous

- Expect there to be some finite relaxation time when a heterogeneous material is suddenly deformed.



- It follows that the effective properties of a homogenized material should reflect this time scale.

Peridynamics

- Peridynamics is an extension of solid mechanics to allow long-range interactions and reduced restrictions on continuity.

- Equation of motion:

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{H}} \mathbf{f}(\mathbf{q},\mathbf{x},t)\; dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x},t)$$

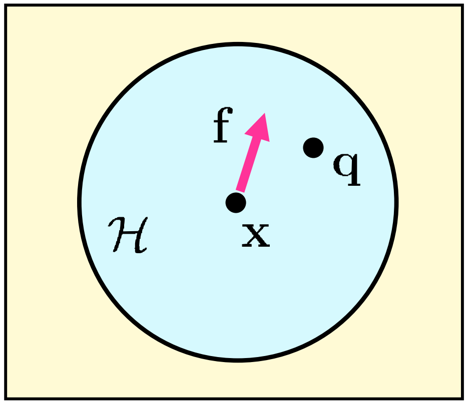
  where ρ=density, $\mathbf{u}$=displacement, $\mathbf{b}$=body force density, and $\mathcal{H}$ is an interaction volume.

- $\mathbf{f}$ is determined by the deformation through a constitutive model.

- Linearized equation of motion (elastic):

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{H}} \mathbf{C}(\mathbf{x},\mathbf{q})(\mathbf{u}(\mathbf{q},t) - \mathbf{u}(\mathbf{x},t))\; dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x},t)$$

  where $\mathbf{C}$ is the *micromodulus* tensor field.



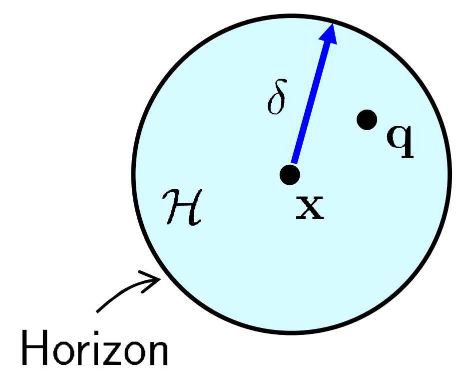
Peridynamics always has a length scale. Does it always have a time scale?

- If $\mathcal{H}$ is bounded, its size provides a length scale (the *horizon*).
- The theory is clearly nonlocal in space.
- We could include nonlocality in time:

$$\rho \ddot{\mathbf{u}} = \int_0^\infty \int_{\mathcal{H}} \mathbf{C}(\mathbf{x}, \mathbf{q}, t - t')) \big(\mathbf{u}(\mathbf{q}, t') - \mathbf{u}(\mathbf{x}, t') \big) \; dV_{\mathbf{q}} \; dt'$$

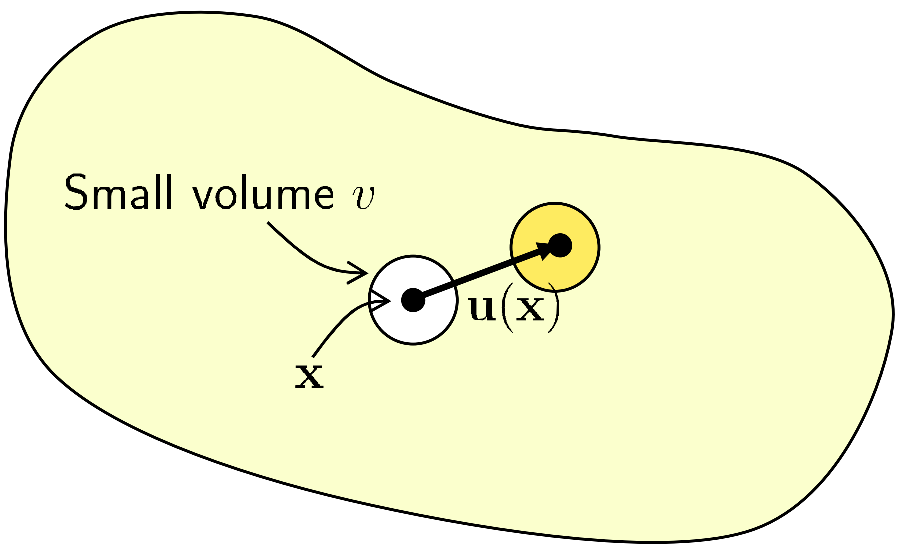
  in which $\mathbf{C}$ has some time scale.

- Does the length scale of $\mathcal{H}$ imply an inherent *material time scale* in an *elastic* material?



To find a material time scale: Find the restoring force on a small volume

- Suppose we displace a small volume v of radius ϵ surrounding a point $\mathbf{x}$ through a distance $\mathbf{u}(\mathbf{x})$ while holding the rest of the body fixed.
- $\epsilon \ll \delta$.
- Find the force $\mathbf{F}$ on v.



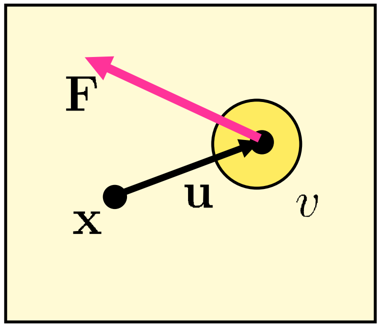
Restoring force on the small volume

- The restoring force on v is

$$\begin{aligned}\mathbf{F} &\approx v\int_{\mathcal{H}} \mathbf{C}(\mathbf{q})\big(\mathbf{u}(\mathbf{q})-\mathbf{u}(\mathbf{x})\big)\,dV_{\mathbf{q}}\\ &= v\int_{\mathcal{H}} \mathbf{C}(\mathbf{q})(\mathbf{0}-\mathbf{u}(\mathbf{x}))\,dV_{\mathbf{q}}\\ &= -v\mathbf{P}(\mathbf{x})\mathbf{u}(\mathbf{x})\end{aligned}$$

  where the *reaction tensor* at $\mathbf{x}$ is defined by

$$\mathbf{P}(\mathbf{x}) = \int_{\mathcal{H}} \mathbf{C}(\mathbf{q})\,dV_{\mathbf{q}}.$$



- $\mathbf{P}$ is symmetric.

Displace the small volume, then let it go

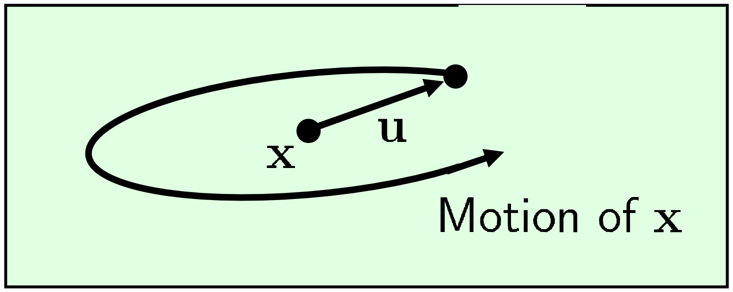
- Newton's second law applied to v:

$$\rho v \ddot{\mathbf{u}}(\mathbf{x},t) = \mathbf{F} = -v\mathbf{P}(\mathbf{x})\mathbf{u}(\mathbf{x},t)$$

  or

$$\rho \ddot{\mathbf{u}}(\mathbf{x},t) = -\mathbf{P}(\mathbf{x})\mathbf{u}(\mathbf{x},t)$$

- (We could have gotten this directly from the equation of motion $\rho\ddot{\mathbf{u}} = \mathbf{L} + \mathbf{b}$.)



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Each point is a linear oscillator (holding other points fixed)

- Assume $\mathbf{u} = a\mathbf{n}e^{i\omega t}$ for some constants ω, a and unit vector $\mathbf{n}$. Use $\rho\ddot{\mathbf{u}} = -\mathbf{P}(\mathbf{x})\mathbf{u}$.

$$-\rho\omega^2 a\mathbf{n}e^{i\omega t} = -a\mathbf{P}(\mathbf{x})\mathbf{n}e^{i\omega t}$$

$$\rho\omega^2\mathbf{n} = \mathbf{P}(\mathbf{x})\mathbf{n}$$

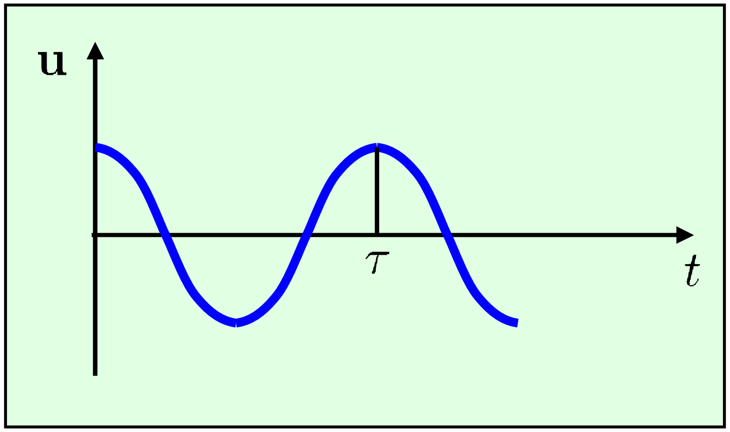
- So $\rho\omega^2$ is an eigenvalue of $\mathbf{P}(\mathbf{x})$ with eigenvector $\mathbf{n}$.
- Can show $\mathbf{P}(\mathbf{x})$ is symmetric. Let P_0 be its smallest eigenvalue.
- Solve for ω:

$$\omega_0 = \sqrt{\frac{P_0}{\rho}}$$

- Define a *material time scale* by

$$\tau := \frac{1}{\omega_0}.$$

- This time scale is independent of a, v.



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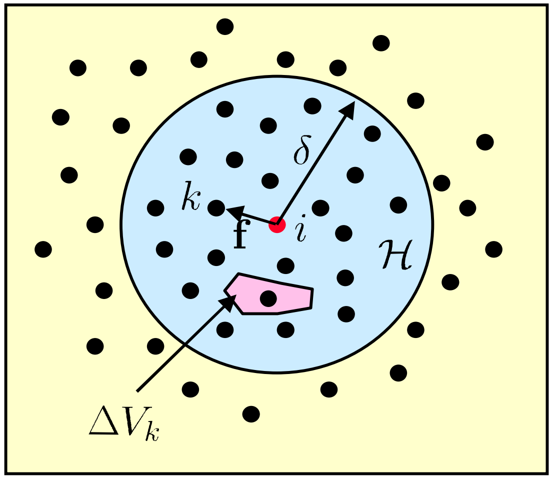
Properties of the peridynamic time scale: Numerical stability

- In the Emu (or PD-LAMMPS) discretization, the numerical stability restriction* on the time step with velocity Verlet time integration is

$$\Delta t \leq \sqrt{2}\,\tau$$

provided $\tau > 0$.

- This is independent of Δx.
- The horizon provides the length scale instead of the discretization.

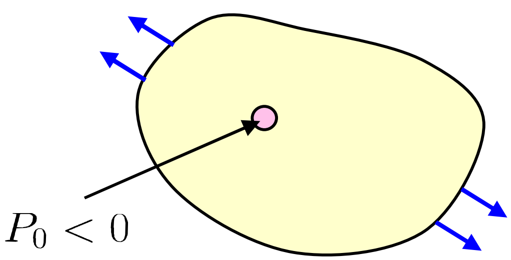


$$\int_{\mathcal{H}} \mathbf{C}(\mathbf{x},\mathbf{q})(\mathbf{u}(\mathbf{q})-\mathbf{u}(\mathbf{x}))\, dV_{\mathbf{q}} \approx \sum_{k\in\mathcal{H}_i} \mathbf{C}(\mathbf{x}_k,\mathbf{x}_i)(\mathbf{u}_k-\mathbf{u}_i)\Delta V_k$$

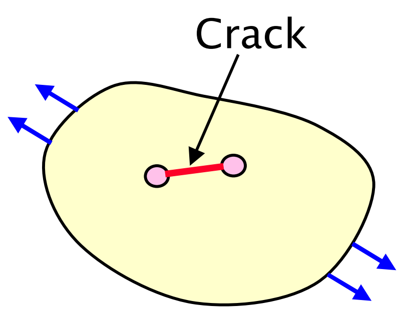
* SS and Askari, *Computers and Structures*, 2005.

Properties of the peridynamic time scale: Material stability

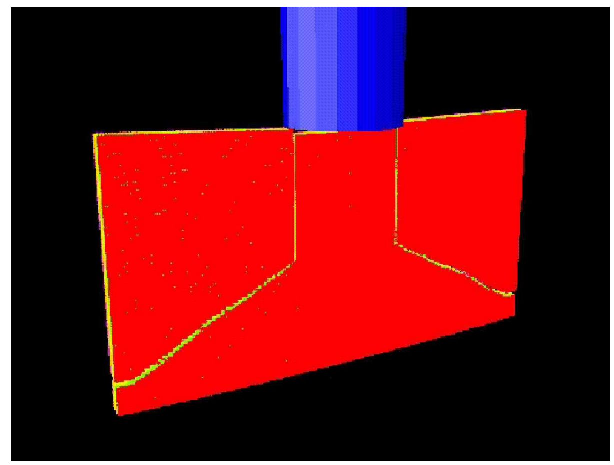
- If any of the eigenvalues of $\mathbf{P}$ are negative, small discontinuities can grow over time.
- This is a "crack nucleation condition*" (something like loss of ellipticity).
- Since $\tau = \sqrt{\rho/P_0}$ can get crack nucleation if the material has an "imaginary material time scale."



Crack nucleation



Crack growth



Nucleation and growth simulation (Emu)

* SS, Weckner, Bobaru, and Askari, *Intl. J. Frac.*, 2010 (to appear).

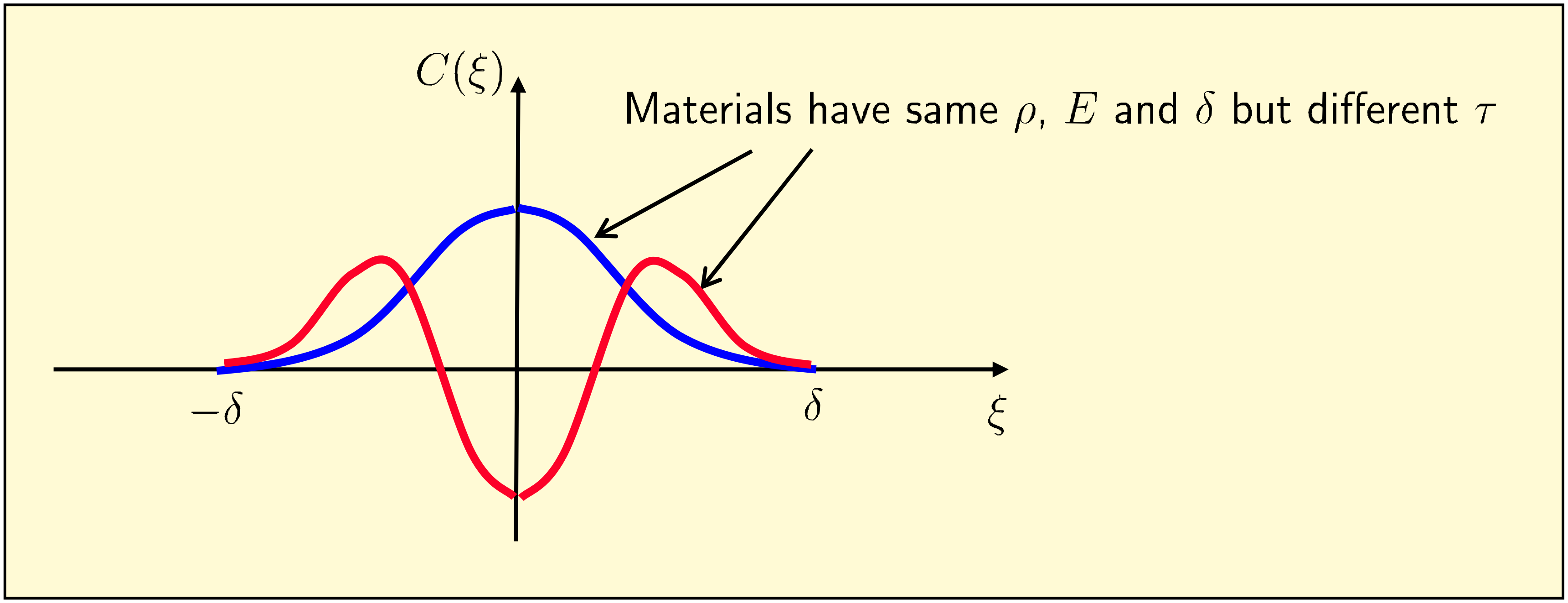
Time scale is not uniquely determined by the length scale and elastic modulus

- Young's modulus (1D):

$$E = \frac{1}{2}\int_{-\delta}^{\delta} \xi^2 C(\xi)\, d\xi$$

- Time scale:

$$\tau = \sqrt{\frac{\rho}{\int_{-\delta}^{\delta} C(\xi)\, d\xi}}$$



Simple rescaling of the horizon

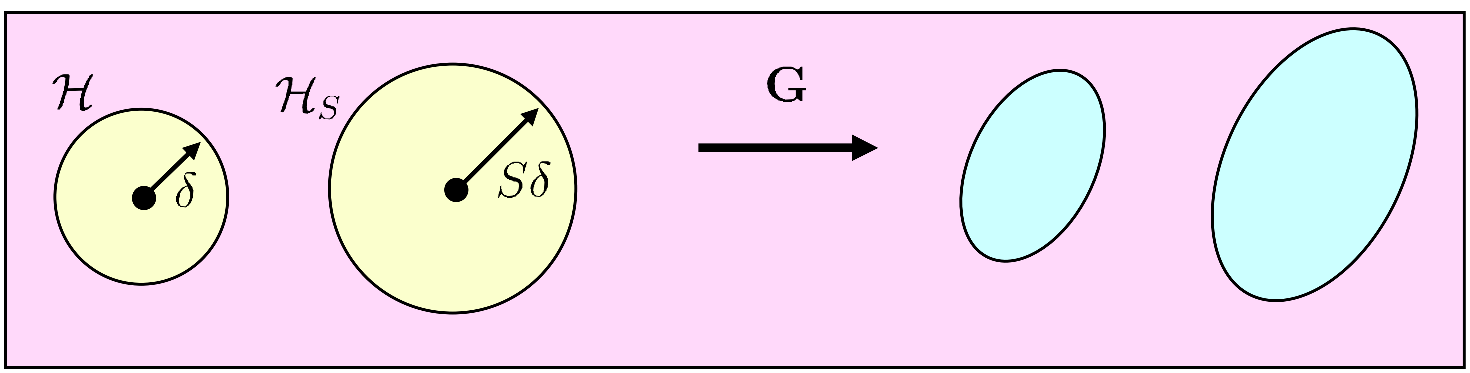
- Let δ be the horizon for a given material. Consider a family of linear elastic materials parameterized by a number $S > 0$, such that

  1. The horizon of each material is $S\delta$, and
  2. The strain energy density under any homogeneous deformation $\mathbf{u}(\mathbf{x}) = \mathbf{G}\mathbf{x}$ is independent of S, where $\mathbf{G}$ is any tensor.

- Try to find $\mathbf{C}^S$ such that

$$W^S = \frac{1}{2}\int_{\mathcal{H}_S} (\mathbf{G}\boldsymbol{\xi}) \cdot \left[\mathbf{C}^S(\boldsymbol{\xi})(\mathbf{G}\boldsymbol{\xi})\right] \, dV_{\boldsymbol{\xi}}$$

does not depend on S.



Relate time scale to a length scale

- Change of dummy variable $\boldsymbol{\xi} = S\boldsymbol{\sigma}$:

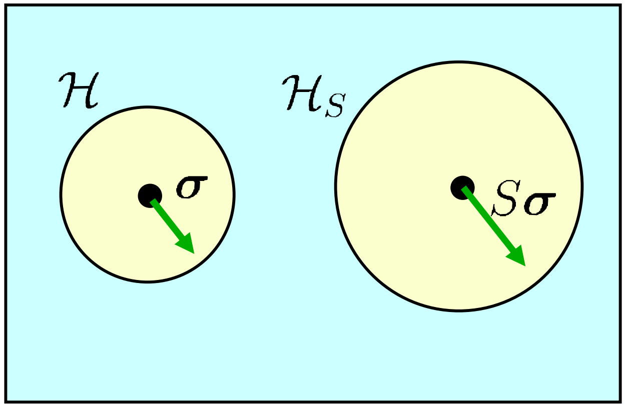
$$2W^S = \int_{\mathcal{H}_S} (\mathbf{G}\boldsymbol{\xi}) \cdot \left[\mathbf{C}^S(\boldsymbol{\xi})(\mathbf{G}\boldsymbol{\xi})\right] \, dV_{\boldsymbol{\xi}} = \int_{\mathcal{H}} (\mathbf{G}S\boldsymbol{\sigma}) \cdot \left[\mathbf{C}^S(S\boldsymbol{\sigma})(\mathbf{G}S\boldsymbol{\sigma})\right] \, (S^3 dV_{\boldsymbol{\sigma}})$$

- The requirement $W^S = W$ therefore leads to

$$\mathbf{C}^S(S\boldsymbol{\sigma}) = S^{-5}\mathbf{C}(\boldsymbol{\sigma}).$$

- Similarly, $\mathbf{P}^S := \int_{\mathcal{H}_S} \mathbf{C}^S(\boldsymbol{\xi}) \, dV_{\boldsymbol{\xi}}$ leads to

$$\mathbf{P}^S = S^{-2}\mathbf{P}.$$



- We now know how $\mathbf{P}^S$ scales with the size of the interaction region δ.

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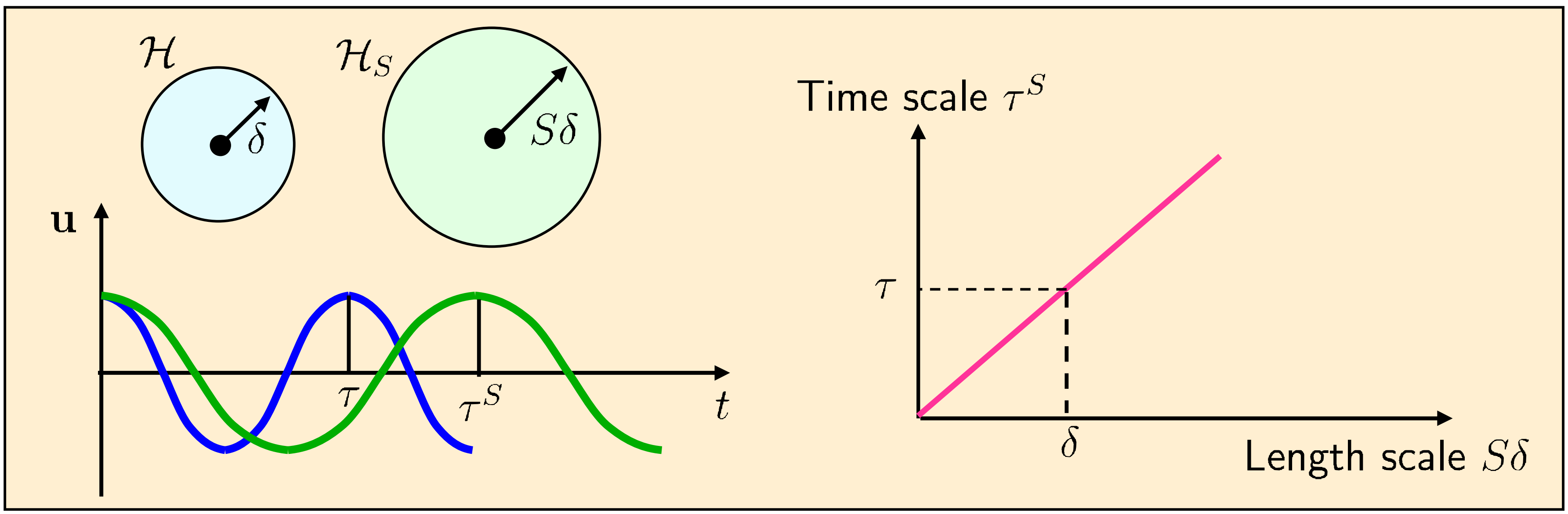
Relate time scale to a length scale, ctd.

- The eigenvalues of $\mathbf{P}^S$ must scale the same way:

$$P_0^S = S^{-2} P_0$$

- so the material time scale is

$$\tau^S := \sqrt{\frac{\rho}{P_0^S}} = \sqrt{\frac{\rho}{S^{-2} P_0}} = S\tau$$



Scaling of dispersion curves under simple rescaling of the horizon

- Linear waves (1D): assume $u = e^{i(\kappa x - \omega t)}$, substitute this into to the equation of motion

$$\rho \ddot{u} = \int_{-\infty}^{\infty} C(\xi)(u(x+\xi) - u(x))\, d\xi$$

so the dispersion curve is determined by

$$\rho\omega^2(\kappa) = \int_{-\infty}^{\infty} C(\xi)\left(1 - e^{i\kappa\xi}\right)\, d\xi$$

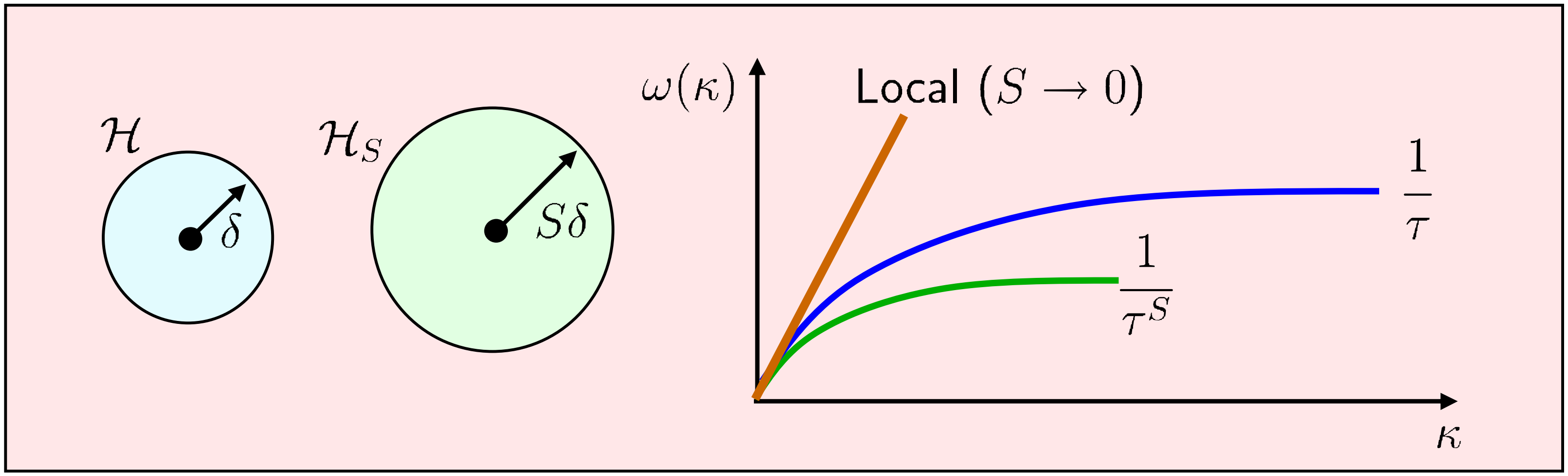
Scaling of dispersion curves, ctd.

- Now repeat this using the C^S and set $\xi = S\sigma$:

$$\begin{aligned}\rho\omega_S^2(\kappa) &= \int_{-\infty}^{\infty} C^S(\xi)\big(1 - e^{i\kappa\xi}\big)\, d\xi \\ &= \int_{-\infty}^{\infty} \big(S^{-3}C(\sigma)\big)\big(1 - e^{i\kappa(S\sigma)}\big)\, (S d\sigma) = S^{-2}\rho\omega^2(S\kappa)\end{aligned}$$

hence the dispersion curve scales according to

$$\omega_S(\kappa) = S^{-1}\omega(S\kappa) \to \frac{1}{\tau^S} \text{ as } \kappa \to \infty.$$



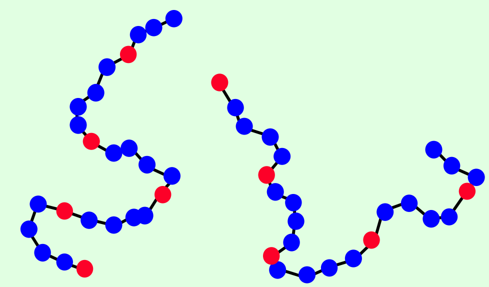
Another way to change length scales: Coarsening*

- We arbitrarily chose a certain way to rescale the material properties:

$$\mathbf{C}^S(\boldsymbol{\xi}) = S^{-5}\mathbf{C}(\boldsymbol{\xi}/S)$$

  which implicitly scales the microstructure ($S > 1$ means "big atoms").

- Now propose an alternative called *coarsening*.
- Start with a detailed description (level 0).
- Choose a coarsened subset (level 1).
- Model the system using only the coarsened DOFs
- Forces on the coarsened DOFs depend only on their own displacements.
- These forces should be the same as you would get from the full detailed model.



Small-scale MD model
Blue: Level 0
Red: Level 1

* SS, *Intl. J. Multiscale Comp. Engin.*, 2010 (to appear).

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Discussion

- "Automatic" increase in τ as the interaction distance increases suggests that within peridynamics, multiscale in space may imply multiscale in time.